

# Hyperfine structure of $S$ states in Li and $\text{Be}^+$

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A large-scale configuration-interaction (CI) calculation is reported for the hyperfine splitting of the  $2^2S$  and  $3^2S$  states of  $^7\text{Li}$  and  $^9\text{Be}^+$ . The CI calculation based on the Dirac-Coulomb-Breit Hamiltonian is supplemented with a separate treatment of the QED, nuclear-size, nuclear-magnetization distribution, and recoil corrections. The nonrelativistic limit of the CI results is in excellent agreement with variational calculations. The theoretical values obtained for the hyperfine splitting are complete to the relative order of  $\alpha^2$  and improve upon results of previous studies.

PACS numbers: 31.15.Ar, 32.10.Fn, 31.30.Gs

The hyperfine structure (hfs) of few-electron atoms has been an attractive subject of theoretical studies for decades, one of the reasons being a few ppm accuracy achieved in experiments on Li and  $\text{Be}^+$  [1, 2]. Interest in this topic was enhanced even further recently, in view of prospects of using hfs data to get an access to the neutron halo structure, the proton charge distribution, and the nuclear vector polarizability, particularly for isotopes of  $\text{Be}^+$  [3, 4]. Despite the considerable attention received, a high-precision theoretical description of hfs in few-electron atoms remains a difficult task. The main problem lies in the high singularity of the hfs interaction and, as a consequence, in the dependence of the calculated results on the quality of the correlated wave function near the nucleus.

Among numerous theoretical investigations performed previously for Li and  $\text{Be}^+$ , two apparently most accurate ones are the multiconfigurational Dirac-Fock (MCDF) calculation [5] and the Hylleraas-type variational calculation [6]. Both studies report good agreement with the experiment, but they are not entirely consistent with each other in treatment of individual corrections. The MCDF calculation does not include the binding QED effects and, in the case of Li, the nuclear magnetization distribution effect. The variational calculation yields accurate results for the nonrelativistic Fermi contact term but treats the relativistic effects in an effective way only, by rescaling the hydrogenic result. This indicates that neither of these studies is complete at the relative order of  $\alpha^2$  ( $\alpha$  is the fine-structure constant). The aim of the present investigation is to perform a high-precision calculation of the hfs splitting in Li and  $\text{Be}^+$ , with a complete treatment of all corrections  $\sim \alpha^2$ .

A possible way to accomplish this task would be to supplement the nonrelativistic calculation [6] with a rigorous evaluation of the relativistic correction, whose expression was recently derived by Pachucki [7]. Such a calculation has not been performed so far. In the present work, the relativistic correction will be accounted for by means of the Dirac-Coulomb-Breit Hamiltonian.

The magnetic dipole hfs splitting of an energy level of an  $nS$  state is conveniently represented in terms of a

dimensionless function  $G_n(Z)$  defined as [8]

$$\Delta E_n = \frac{4}{3} \frac{\alpha(Z\alpha)^3}{n^3} \frac{m}{m_p} \frac{\mu}{\mu_N} \frac{2I+1}{2I} \frac{mc^2}{(1+m/M)^3} G_n(Z), \quad (1)$$

where  $\mu$  is the nuclear magnetic moment,  $\mu_N = |e|/(2m_p)$  is the nuclear magneton;  $m$ ,  $m_p$ , and  $M$  are the masses of the electron, the proton, and the nucleus, respectively;  $I$  is the nuclear spin quantum number, and  $Z$  is the nuclear charge number. The function  $G$  defined in this way is unity for a non-relativistic point-nucleus H-like atom.

Within the leading relativistic approximation, the electron correlation can be described by the Dirac-Coulomb-Breit equation, which is solved by the configuration-interaction (CI) Dirac-Fock (DF) method in the present work. The many-electron wave function  $\Psi(PJM)$  with the parity  $P$ , the momentum quantum number  $J$ , and the momentum projection  $M$  is represented as a sum of configuration-state functions (CSFs),

$$\Psi(PJM) = \sum_r c_r \Phi(\gamma_r PJM). \quad (2)$$

The CSFs are obtained as linear combinations of the Slater determinants constructed from the positive-energy solutions of the Dirac equation with the frozen-core DF potential. The mixing coefficients  $c_r$  are determined by diagonalizing the Hamiltonian matrix. The hfs splitting is obtained as the expectation value of the hfs operator on the many-electron wave function (2). The corresponding formulas are well-known, see, *e.g.*, [5]. To perform a CI calculation, we devised a code, incorporating and adapting a number of existing packages [9] for setting up the CSFs, calculating angular-momentum coefficients, and diagonalizing the Hamiltonian matrix. The largest number of CSFs simultaneously handled was about a half of a million, with the number of nonzero elements in the Hamiltonian matrix of about 5 billions. A thorough optimization of the code was carried out, in order to keep the time and memory consumption of the calculation within reasonable limits.

The dominant part of the hfs splitting in light atoms is delivered by the Dirac-Coulomb Hamiltonian. This

TABLE I: The Dirac-Coulomb-Breit part of the hfs splitting, in terms of  $G(Z)$ .

	$l_{\max}$	Li $2^2S$	Be $^+$ $2^2S$
Coulomb	1	0.214 470 3	0.390 159 9
	2	0.215 167 8	0.390 798 6
	3	0.215 304 4	0.390 938 7
	4	0.215 346 2	0.390 984 7
	5	0.215 362 9	0.391 003 8
	6	0.215 371 9	0.391 014 5
	7	0.215 376 5	0.391 020 2
	$\infty$	0.215 384 8(49)	0.391 030 4(61)
Breit		0.000 015 9	0.000 038 6
Total		0.215 400 7(49)	0.391 069 0(61)
MCDF [5]		0.215 287	0.390 984
Hylleraas <sup>a</sup> [6]		0.215 379(13)	0.391 023(34)

<sup>a</sup> the sum of the nonrelativistic, the relativistic, and the nuclear-charge distribution terms.

was the most demanding part of the calculation since a high relative precision was required. The one-electron orbitals for constructing CFSs were obtained by the dual-kinetic-balance (DKB) B-spline basis set method [10] for the Dirac equation. For a given number of B-splines  $n_a$ , all eigenstates were taken with the energy  $0 < \varepsilon \leq mc^2(1 + Z\alpha E_{\max})$  and the orbital quantum number  $l \leq l_{\max}$ , where  $E_{\max}$  was varied between 0.5 and 6 and  $l_{\max}$ , between 1 and 7. Three main sets of one-electron orbitals were employed in the present work: (A)  $20s\ 20p\ 19d\ 19f\ 18g\ 18h$  with  $n_a = 44$  and  $E_{\max} = 3$ , (B)  $14s\ 14p\ 14d\ 13f\ 13g\ 13h\ 12i\ 12k$  with  $n_a = 34$  and  $E_{\max} = 0.5$ , and (C)  $25s\ 25p\ 24d$  with  $n_a = 54$  and  $E_{\max} = 6$ . Here, the notation, *e.g.*,  $20p$  means  $20p_{1/2}\ 20p_{3/2}$ . Calculational results were first obtained with the set (A) and then corrected for contributions of the higher partial waves with the set (B) and for a more complete representation of the Dirac spectrum with the set (C). The set of CSFs used in the calculation was obtained by taking all single, double, and triple excitations from the reference configuration with at least one electron orbital with  $l \leq 1$  present. The triple excitations that were left out in this way were found to yield a negligible contribution. Inclusion of the *Breit interaction* into the Dirac-Coulomb Hamiltonian yields only a small correction in the case of Li and Be $^+$ . Since the effect is small, it is sufficient to use a much shorter basis set for its evaluation, which simplifies the computation greatly.

The results of our CI calculation of the Dirac-Coulomb-Breit part of the ground-state hfs in  $^7\text{Li}$  and  $^9\text{Be}^+$  are presented in Table I. The Fermi model was employed for the nuclear-charge distribution, with the nuclear-charge radii [11]  $\langle r^2 \rangle^{1/2} = 2.431(28)$  fm for Li and  $\langle r^2 \rangle^{1/2} = 2.518(11)$  fm for Be. The uncertainties specified in the table include the estimated error due to the incompleteness of the basis and due to the finite nuclear size. The error of the Breit part was found to be negligible. Our results are in reasonable agreement with the nonrelativistic variational results [6] but deviate signifi-

cantly from the MCDF values [5]. The comparison leads us to a conclusion that the dominant part of the relativistic correction can indeed be accounted for by an effective scaling of the hydrogenic results, as was argued in [6]. A complete evaluation of the relativistic correction within the  $Z\alpha$ -expansion approach, however, has to be performed along the way paved in [7], which has not been done yet.

Comparison with the results of [6] would become possible on a much higher level of accuracy if we identified the nonrelativistic part of our CI results. Such an identification was carried out by repeating our CI calculations for different values of  $\alpha$  (namely, three values with ratios  $\alpha'/\alpha = 0.9, 1$ , and  $1.1$  were used). For each value of  $\alpha$ , the finite nuclear-charge distribution (FNC) correction was evaluated separately and subtracted from the CI values. The point-nucleus results thus obtained were fitted to a polynomial in  $\alpha$ , assuming the absence of the linear term. In this way, the CI results with the physical value of  $\alpha$  were separated into three parts: the nonrelativistic point-nucleus contribution, the relativistic point-nucleus correction, and the FNC correction. The numerical results for them are listed in Table II.

The *FNC correction* was evaluated for both the hydrogenic wave functions and the CI many-electron wave functions. In the latter case, a series of the CI calculations with different values of the nuclear-charge radius  $R$  was performed and the FNC correction was extracted by a fit, using the analytical form of the  $R$  dependence [8]. It was found that, with an accuracy of  $\sim 0.5\%$ , there was no screening effect on the relative value of this correction.

The *QED effects* induce the largest correction to be added to the Dirac-Coulomb-Breit hfs value. For  $nS$  states of few-electron atoms, the QED correction can be written in the same form as for hydrogen [15],

$$\delta G_n(Z) = \frac{\alpha}{\pi} G_n^{\text{NR}}(Z) \left\{ \frac{1}{2} + Z\alpha\pi \left( \ln 2 - \frac{5}{2} \right) + (Z\alpha)^2 \left[ -\frac{8}{3} \ln^2(Z\alpha) + a_{21} \ln(Z\alpha) + a_{20} \right] \right\}, \quad (3)$$

where  $G_n^{\text{NR}}$  is the nonrelativistic hfs value. The first three coefficients in the  $Z\alpha$  expansion (3) are the same as for hydrogen. The higher-order terms  $a_{21}$  and  $a_{20}$  are different and not known at present. One can, however, estimate them with their hydrogenic values [16, 17]:  $a_{21}(2s) = -1.1675$ ,  $a_{20}(2s) = 11.3522$ ,  $a_{21}(3s) = -2.3754$ , and  $a_{20}(3s) = 9.7474$ . A 100% uncertainty is ascribed to this approximation. Essentially the same treatment of the QED correction was reported in [6]; the QED results of [5] differ by  $\sim 40\%$  due to the neglect of the binding QED effects [i.e., the terms in (3) beyond the first one].

The *nuclear structure effects* have significant influence on hfs and should be taken into account. Their rigorous description is a demanding problem. The way for its solution was paved in recent studies [4, 18]. Practical realizations of this approach, however, are so far restricted by two- and three-nucleon systems [18] and their

TABLE II: Individual contributions to the hfs splitting, in terms of  $G(Z)$ . The experimental values for the function  $G$  for Li were inferred from the original references by using the nuclear magnetic moment  $\mu/\mu_N = 3.256\,426\,8(17)$  [12].

	${}^7\text{Li } 2^2S$	${}^7\text{Li } 3^2S$	${}^9\text{Be}^+ 2^2S$	${}^9\text{Be}^+ 3^2S$
Nonrelativistic	0.215 251 <sup>a</sup>	0.168 340 <sup>a</sup>	0.390 544 <sup>a</sup>	0.335 066 <sup>a</sup>
Ref. [6]	0.215 254 (4)	0.168 351 (13)	0.390 549 (9)	
Relativistic	0.000 205 <sup>a</sup>	0.000 159 <sup>a</sup>	0.000 664 <sup>a</sup>	0.000 564 <sup>a</sup>
Finite nuclear charge	-0.000 055 <sup>a</sup>	-0.000 043 <sup>a</sup>	-0.000 139 <sup>a</sup>	-0.000 119 <sup>a</sup>
Dirac-Coulomb-Breit	0.215 401 (5)	0.168 456 (9)	0.391 069 (6)	0.335 510 (9)
QED	0.000 182 (4)	0.000 143 (4)	0.000 289 (12)	0.000 250 (12)
Bohr-Weisskopf	-0.000 024 (3)	-0.000 019 (2)	-0.000 062 (17)	-0.000 053 (14)
Specific mass shift	0.000 002	0.000 002	0.000 002	0.000 002
Negative-continuum	0.000 002	0.000 002	0.000 005	0.000 005
Total theory	0.215 563 (7)	0.168 584 (10)	0.391 304 (22)	0.335 714 (21)
Ref. [6]	0.215 54 (2)	0.168 58 (2)	0.391 27 (4)	
Experiment	0.215 561 1 (1) <sup>b</sup>	0.168 60 (2) <sup>c</sup>	0.391 260 (1) <sup>e*</sup>	
		0.171 5 (4) <sup>d</sup>	0.391 240 (6) <sup>e†</sup>	

<sup>a</sup> These three entries are inferred from the corresponding Dirac-Coulomb-Breit values; their sum is expected to be more accurate than each of the entries separately; <sup>b</sup> Ref. [1]; <sup>c</sup> Ref. [13]; <sup>d</sup> Ref. [14]; <sup>e\*</sup> Ref. [2] with  $\mu/\mu_N = -1.177\,432(3)$  [12]; <sup>e†</sup> Ref. [2] with  $\mu/\mu_N = -1.177\,49(2)$  [12].

extension for more complex nuclei like  ${}^7\text{Li}$  and  ${}^9\text{Be}$  looks problematic.

The most widely used approach up to now is to account for the nuclear magnetization distribution [the Bohr-Weisskopf (BW) effect] by means of the Zemach formula [19], which is simple and apparently model independent. Such approach ignores inelastic effects, which can yield a large contribution [18], and it is not clear what uncertainty should be ascribed to such results. In the present study, we calculate the BW correction within the single-particle (SP) nuclear model [20, 21], in which the nuclear magnetic moment is assumed to be induced by the odd nucleon. This model is expected to be reasonably adequate for  ${}^7\text{Li}$  since it reproduces well the observable nuclear magnetic moment basing on just the free-nucleon  $g$  factors, the difference being only 15%. For  ${}^9\text{Be}$ , the deviation is four times larger and the SP approach is expected to yield worse results.

Within the SP model, the BW effect can be accounted for by adding a multiplicative magnetization-distribution function to the standard point-dipole hfs interaction [21]. The distribution function is induced by the wave function of the odd nucleon and is obtained by solving the Schrödinger equation with the Woods-Saxon potential and an empirical spin-orbit interaction included. The parameters of the potential were taken from [22]. The BW correction was calculated for both the one-electron wave functions and the CI many-electron wave functions. It was found that, with a very good accuracy ( $< 0.5\%$ ), there was no screening effect on the relative value of this correction. Our calculational results are larger than the Zemach-formula values of [6] by  $\sim 10\%$  in the case of Li and by  $\sim 30\%$  in the case of Be. The Zemach-formula result of [5] for Be is larger than the one of [6] by a factor of four, which is due, we believe, to a misinterpretation of the Zemach formula in [5]. Our computational results for the BW correction are presented in Table II. The error

bars specified were obtained as the difference of the SP and the Zemach values and should be regarded as order-of-magnitude estimations of the error. We checked that similar evaluations of the nuclear effect on hfs in  ${}^3\text{He}^+$  agree well with a much more elaborate calculation of [18].

The leading *recoil* contribution is given by the mass scaling factor  $(1+m/M)^{-3}$  included into the definition of the function  $G$  in (1). The remaining correction (within the nonrelativistic approach) is due to the specific mass shift (SMS) and is very small for the  $S$  states. We calculate it by introducing the SMS term  $(m/M) \sum_{i<j} \mathbf{p}_i \cdot \mathbf{p}_j$  into the Dirac-Coulomb Hamiltonian and taking the increment of the CI results with and without SMS ( $\mathbf{p}$  is the momentum operator). Our results agree with the estimates obtained in [6] but are more accurate. For the  $2^2S$  and  $3^2S$  states of Li, we obtain  $\delta G = 2.0(2) \times 10^{-6}$  and  $1.9(2) \times 10^{-6}$ , respectively, which should be compared with  $2(5) \times 10^{-6}$  and  $2(20) \times 10^{-6}$  from [6], respectively.

The *negative-continuum contribution* might be of some importance in calculations involving the operators that mix the upper and the lower components of the Dirac wave function. The hfs operator is of this kind, so we have to obtain an estimation for this correction. We calculate the negative-continuum contribution by employing the many-body perturbation theory to the first order. The same one-electron DKB basis set was used as in the CI calculations, with the only difference that all negative-energy eigenstates were taken.

Our total theoretical values for the hfs splitting presented in Table II agree with the results by Yan *et al.* [6] but are more accurate. The present theory agrees very well with experiments on Li, the only exception being the experimental result [14], which contradicts both the theory and the result of a more recent measurement [13]. The comparison of theoretical calculations with the high-precision experiment for the ground state of  $\text{Be}^+$

[2] is complicated by the existence of two different values for the nuclear magnetic moment [12]. The smaller value yields a better agreement with our theoretical result, but there is still a  $2\sigma$  deviation present. Having in mind that the experimental results for the magnetic moment are in significant disagreement with each other, one can surmise the presence of underestimated systematic effects in one or both of these measurements. We thus employ the comparison presented in Table II to infer an independent value of the magnetic moment, which reads  $\mu(^9\text{Be})/\mu_N = -1.177\,30(6)$  and is somewhat smaller than the both values from [12].

In summary, we have performed a large-scale CI calculation of the hfs splitting of the  $2^2S$  and  $3^2S$  states of Li and  $\text{Be}^+$ . The results obtained from the Dirac-Coulomb-Breit Hamiltonian agree with the previously

reported nonrelativistic values but are more accurate due to a rigorous treatment of the relativistic correction. The QED, nuclear magnetization distribution, recoil, and negative-continuum corrections were evaluated separately and added to the Dirac-Coulomb-Breit value. Detailed comparison with the earlier calculations were made and some inconsistencies in their previous treatment of individual corrections were revealed. The calculational results for Li are in good agreement with the experimental data. For  $\text{Be}^+$ , the theoretical prediction deviates from the experimental value by 2 or  $3\sigma$ , depending on the value of the nuclear magnetic moment used.

Krzysztof Pachucki is gratefully acknowledged for suggesting the topic of this investigation and valuable discussions. The work was supported by the RFBR grant no. 06-02-04007 and by the foundation “Dynasty”.

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